MODELING OF COAL CONVERSION PROCESSES IN FIXED BEDS

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Abstract

An advanced, one-dimensional fixed-bed coal gasification and combustion model is presented. The model considers separate gas and solid temperatures, axially variable solid and gas flow rates, variable bed void fraction, coal drying, devolatilization based on functional groups and depolymerization, vaporization and cross-linking, oxidation and gasification of char, and partial equilibrium in the gas phase. The model is described by 191 highly non-linear, coupled, first order differential equations. Due to the countercurrent nature of the gas and solids flow the system of equations constitutes a split-boundary value problem which is solved by converting it to an initial value problem. This paper presents a split back-and-forth shooting technique which exactly satisfies conditions at both the upper and the lower boundary and provides significant improvements in the predictions. Comparisons of the predicted and experimental results for an atmospheric, air-blown Wellman-Galusha gasifier fired with Jetson bituminous coal are presented.

Introduction

Combustion and gasification of coal in fixed beds or slowly moving beds is of great commercial interest as these systems can be integrated into combined cycle processes. In addition, these systems are reliable, require minimal pretreatment of feed coal, offer high thermal efficiencies, and generate easily disposable wastes. Due to these features, the fixed bed systems have been the focus of significant modeling efforts (Amundson and Arri, 1978; Yoon et al., 1978, Desai and Wen, 1978; Earl and Islam, 1985; Thorness and Kang, 1986; Bhattacharya et al., 1986). Most of these models make simplifying assumptions such as equal gas and solid temperatures, plug flow, constant bed porosity, instantaneous devolatilization and use oversimplified gas phase chemistry. More recently, Hobbs et al., (1992) presented a one-dimensional fixed-bed model, MBED-1, in which most of these assumptions were relaxed. A major contribution of their model was the integration of an advanced devolatilization submodel which is based on the functional group composition of the feed coal (Solomon and Hamblen, 1985). This model was combined with a semi-empirical correlation (Ko et al., 1988) for tar evolution. Their simulations showed that the predictions were very sensitive to the potential tar forming fraction of the coal and demonstrated a need for a more rigorous tar evolution submodel. In this paper, an improved model FBED-1 (Fixed-BED, 1-dimensional) is presented. In the FBED-1 model, devolatilization is based on a more rigorous Functional Group, Depolymerization, Vaporization, Crosslinking submodel (FG-DVC) proposed by Solomon et al., (1988). In the FG-DVC submodel, the DVC portion governs the tar evolution and is based on the chemical structure of the coal. In this paper, details relating to FBED-1 model are presented. For details regarding the FG-DVC submodel, the reader is referred to Solomon et al., (1988, 1990).

Conservation Equations

The core of the fixed-bed model, FBED-1, is a set of 191 coupled, first order ordinary differential equations. These equations simulate the chemical and physical processes taking place in both the gas and the solid phases during the coal conversion in a fixed-bed. The conservation equations for mass and energy form the foundation of the FBED-1 model. The gas and solid phase equations are coupled through the source terms. These source terms account for the release of mass from the solid phase to the gas phase, and energy exchange between the two phases. Tar is considered to be a pseudospecies in the FBED-1 formulation. The two-phase conservation equations have been derived by Crowe and Smoot (1979). The set of governing differential equations is listed in Table 1. It is also pointed out that the gas phase species continuity equations are solved only when the gas phase is assumed not to be in chemical equilibrium.

Auxiliary Equations

The set of auxiliary equations for FBED-1 is essentially the same as presented by Hobbs et al., (1992). Since plug flow is assumed for both the solid and the gas phases, the momentum equation is solved to calculate the gas phase pressure drop. Ergun's equation is used to calculate the friction factor and the bed void fraction is assumed to vary linearly between the feed coal and the product ash void fractions. At temperatures higher than a user-specified value, usually 1200 K, the gas phase is assumed to be in chemical and thermal equilibrium and its composition and temperature are computed by Gibbs free energy minimization. The option to keep tar either in or out of chemical equilibrium is provided in FBED-1. The calculation of heat and mass transfer coefficients and transport and thermodynamic properties of gas and tar phases are based on the same correlations as used and discussed by Hobbs et al., (1992).

Solution Methods

Due to the countercurrent flows of gas and solids, the system of governing equations constitutes a split boundary value problem. The input conditions for the solid phase are known at the top of the gasifier, whereas the input conditions for the gas phase are known at the bottom of the gasifier. This system of equations can be converted to an initial value problem and integrated from the top to the bottom of the gasifier, provided the initial estimates for the gas phase quantities are made available at the top of the gasifier. These estimates are made by a zero-dimensional, two-zone, well mixed, partial equilibrium submodel. The zero-dimensional submodel considers drying and devolatilization on one side and gasification and oxidation on the other to take place in separate zones. Its primary use is to provide initial estimates for the product gas enthalpy, composition and species flow rates, as well as the product tar composition and flow rate. Once these estimates are known, the system of equations is integrated from the top to the bottom of the gasifier using LSODE (Livermore Solver for Ordinary Differential Equations, Hindmarsh, 1983) package. Figure 1 shows the predicted results for an atmospheric, air-blown, dry-ash, Wellman-Galusha gasifier fired with Jetson bituminous coal. Experimental results (Thimsen et al., 1984) are also shown. Figure 1 also shows that the boundary conditions for the feed gas stream are not satisfied. The composition of product gas also does not compare well with the experimental data. It overpredicts the amount of H_2O and the product tar flow rate, and underpredicts the amount of O_2 in the feed gas stream, the wall heat loss and the feed gas temperature. Since the feed gas temperature was not reported, it was estimated to be 560 K to allow for the heat exchange between the ash and the feed gas below the gasifier bed. It is pointed out that the gas phase concentrations were determined assuming the gas phase to be in equilibrium in the zero-dimensional submodel. Only marginal improvements were observed in the product gas composition when the devolatilized gases were kept out of equilibrium in the drying and devolatilization zone. The predicted temperature and pressure profiles show the experimentally observed trends. These results clearly indicate a need for an improved solution method.

In order to improve on the FBED-1 predictions and to satisfy the boundary conditions for both the solid and the gas streams, a back-and-forth integration scheme has been developed and implemented. In this scheme, the differential equations are solved from the top to the bottom of the gasifier using the results of the two-zone, zero-dimensional submodel as the initial guess. After the first downward integration pass, the gas phase variables are initialized to the known input conditions. Then the gas phase equations are integrated from the bottom to the top of the gasifier. In the upward integration pass, the solid phase variables are held constant and the solid-gas exchange quantities are calculated from the values predicted during the downward integration pass. This yields a new guess for the gas phase quantities at the top of the gasifier which are then used for the next downward integration sweep. This improves the results and the next downward integration sweep, in which the complete set of equations is integrated, closely satisfies the feed gas boundary conditions except for the temperature. Finally, to satisfy the feed gas temperature, the split back-and-forth integration has been coupled with the shooting method with the product gas enthalpy as the iteration variable. In this scheme, the product gas enthalpy is varied, while all other gas phase quantities are held constant, and the complete set of equations is integrated from the top to the bottom of the gasifier. Once the feed gas temperature is converged within the specified tolerance, an upward pass is taken to compute the final product gas composition and temperature. Convergence is typically obtained in 8-10 iterations.

Figure 2 shows the results obtained using this revised solution method. The solution satisfies the feed gas composition and temperature. The product gas composition, the product tar flow rate and the wall heat loss also show marked improvement and compare well with the experimental data. The predicted pressure profile also compares well with the experimental data. The solid and the gas temperatures profiles show increase in the peak temperatures. This is caused by the higher amount of oxygen and lower amount of H_2O available which lead to higher oxidation rate and thus higher temperatures. The predicted solid temperature profile exceeds the peak measured temperature but compares reasonably well with the experimental data. Finally, the product gas temperature still does not compare well with the experimental data. It should be noted that the reported effluent gas temperature is at the gas-off take location whereas the predicted product gas temperatures is at the gasifier bed top. A proper submodel to account for the heat transfer in the free board zone will improve these predictions.

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Nomenclature

Symbol	*Definition and Units*
A	Cross sectional area of reactor, m^2
D	Diffusivity, m^2/s
h	Enthalpy, J/kg
Q	Heat loss, *watts*
r	Volumetric reaction rate, $kg/m^3\,s$
W	Mass flow rate, kg/s
z	Axial distance, m

Subscripts	*Definition*
d	Devolatilization
g	Gas
gw	Gas-to-wall
i	Index for drying, devolatilization, gasification and oxidation reactions
j	Index for elements C, H, O, N, and S
l	Index for gaseous species
moisture	Moisture
sg	Solid-to-gas
sw	Solid-to-wall

Superscripts	*Definition*
gas	Gas
tar	Tar

Table 1. Governing Equations for FBED-1

Overall Gas Continuity	$$\frac{dW_g}{dz} = A\sum_{i=1}^{6} r_i$$	(1)
Overall Solid Continuity	$$\frac{dW_s}{dz} = -A\sum_{i=1}^{6} r_i$$	(2)
Gas Phase Energy	$$\frac{dW_g h_g}{dz} = A(Q_{sg} - Q_{gw} + \sum_{i=1}^{6} r_i h_{ig})$$	(3)
Solid Phase Energy	$$\frac{dW_s h_s}{dz} = A(-Q_{sg} - Q_{sw} - \sum_{i=1}^{6} r_i h_{ig})$$	(4)
Gas Phase Species Continuity	$$\frac{dW_{g,1}}{dz} = A\sum_{i=l}^{6} r_{i,1}^{gas}$$	(5-26)
Gas Phase Elemental Continuity	$$\frac{dW_{g,j}}{dz} = A\sum_{i=l}^{6} r_{i,1}$$	(27-31)
Overall Tar Continuity	$$\frac{dW_{tar}}{dz} = Ar_d^{tar}$$	(32)
Tar Elemental Continuity	$$\frac{dW_{tar,j}}{dz} = Ar_{d,j}^{tar}$$	(33-37)
Moisture Continuity	$$\frac{dW_{moisture}}{dz} = -Ar_{drying}$$	(38)

Notes:

1. Equations 39-164 describe the FG-DVC devolatilization submodel (Radulovic et al., 1992).
2. Equations 165-191 describe the lower bound of the distribution function for the gas phase tar cracking reactions and follow the FG-DVC formulation (Radulovic et al., 1992).
3. Equations 5-26 are solved only when the gas phase is not considered to be in chemical equilibrium.
4. i=1-6 represents drying, devolatilization, CO_2, H_2, H_2O gasification and oxidation reactions respectively.
5. j=1-5 represents elements C, H, O, N, and S respectively.
6. l=1-22 represents 22 gaseous species considered in FBED-1.

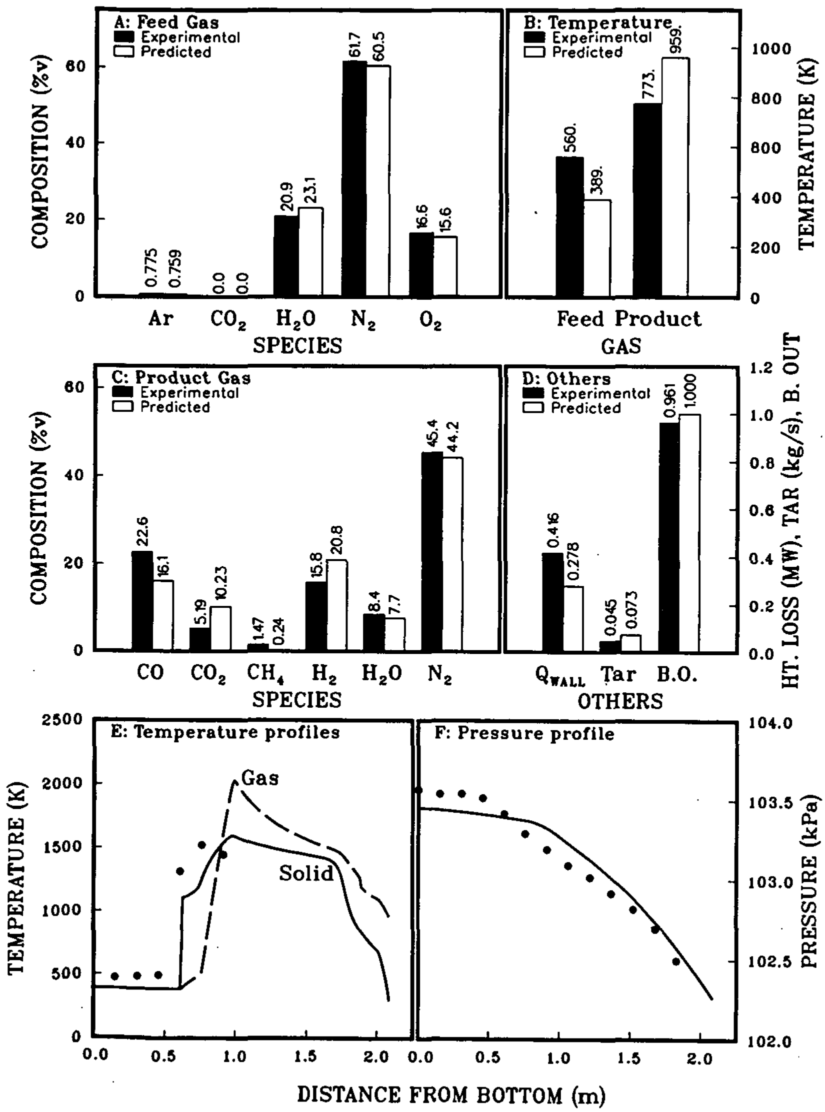

Figure 1. Comparison of predicted and experimental results for an atmospheric, air-blown, dry-ash, Wellman-Galusha gasifier fired with Jetson bituminous coal. The predictions are obtained by converting the system of equations to an initial value problem.

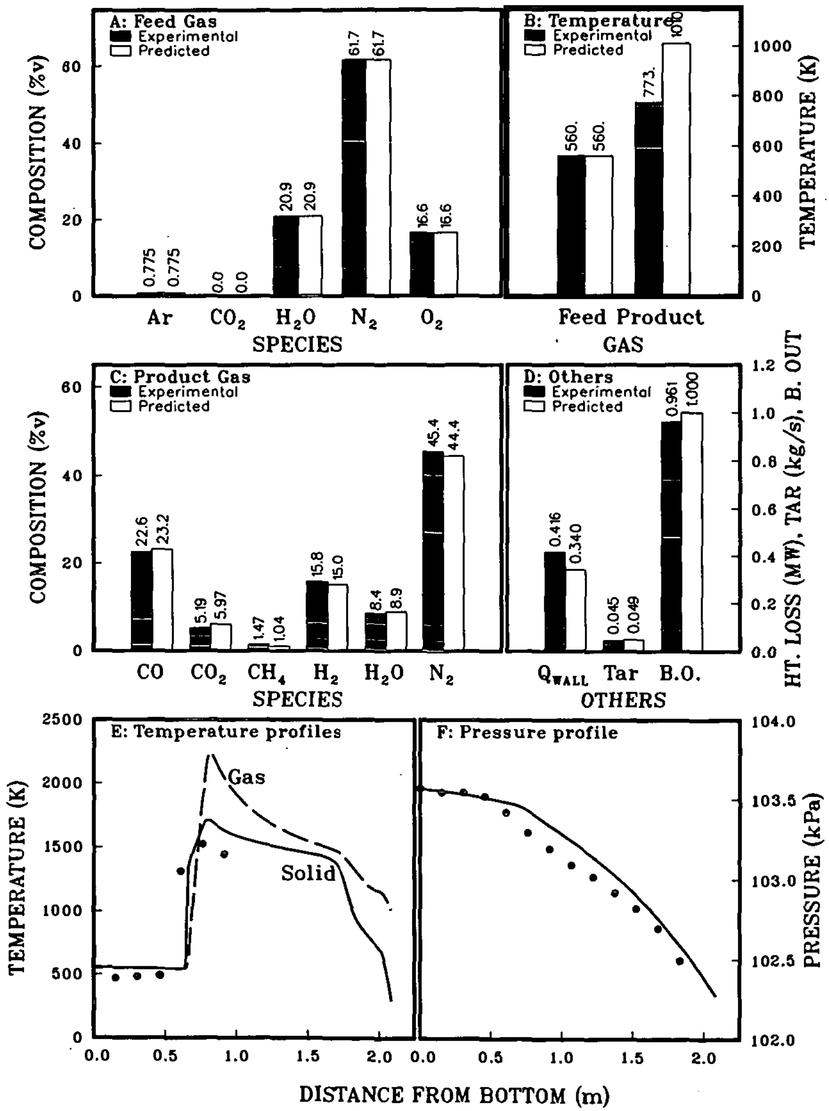

Figure 2. Comparison of predicted and experimental results for an atmospheric, air-blown, dry-ash, Wellman-Galusha gasifier fired with Jetson bituminous coal. The predictions are by a split back-and-forth shooting method.